Accelerating weather models with PGI compilers

The Portland Group
www.pgroup.com

dave.norton@pgroup.com

PGI

CUDA Fortran in 3 slides

CUDA Fortran VADD Host Code

```
subroutine vadd( A, B, C )
  use cudafor
  use kmod
  real, dimension(:) :: A, B
  real, pinned, dimension(:) :: C
  real, device, allocatable:: Ad(:), Bd(:), Cd(:)
  integer :: N
  N = size( A, 1 )
  allocate( Ad(N), Bd(N), Cd(N) )
  Ad = A(1:N)
  Bd = B(1:N)
  call vaddkernel<<<(N+31)/32,32>>>( Ad, Bd, Cd, N )
  C = Cd
  deallocate( Ad, Bd, Cd )
 end subroutine
```

CUDA Fortran VADD Device Code

```
module kmod
 use cudafor
contains
 attributes(global) subroutine vaddkernel(A,B,C,N)
  real, device :: A(N), B(N), C(N)
  integer, value :: N
  integer :: i
  i = (blockidx%x-1)*32 + threadidx%x
  if( i <= N ) C(i) = A(i) + B(I)
 end subroutine
end module
```

Building a CUDA Fortran Program

- CUDA Fortran is supported by the PGI Fortran compilers when the filename uses a CUDA Fortran extension. The .cuf extension specifies that the file is a free-format CUDA Fortran program;
- The .CUF extension may also be used, in which case the program is processed by the preprocessor before being compiled.
- To compile a fixed-format program, add the command line option –Mfixed.
- CUDA Fortran extensions can be enabled in any Fortran source file by adding the –Mcuda command line option.

- Most F2003 features should work in CUDA Fortran.

- There is a (CUDA-like) API to access features
  - Streams supported through API rather then language

Accelerator Directives for flat performance profile codes in 6 slides

Accelerator VADD Device Code

(two dimensional array example)

```
module kmod
 contains
 subroutine vaddkernel(A,B,C)
  real :: A(:,:), B(:,:), C(:,:)
!$acc region
  C(:,:) = A(:,:) + B (:,:)
  <lots of other code to do neat stuff>
  <special code to do even neater stuff>
!$acc end region
 end subroutine
end module
```

!$acc region clauses can surround many individual loops and compute kernels. There is no implicit GPU/CPU data movement within a region

Compiling the subroutine:

```
PGI$ pgfortran -Minfo=accel -ta=nvidia -c vadd.F90

vaddkernel:
    5, Generating copyout(c(1:z_b_14,1:z_b_17))
       Generating copyin(a(1:z_b_14,1:z_b_17))
       Generating copyin(b(1:z_b_14,1:z_b_17))
       Generating compute capability 1.0 binary
       Generating compute capability 1.3 binary
       Generating compute capability 2.0 binary
    6, Loop is parallelizable
       Accelerator kernel generated
        6, !$acc do parallel, vector(16) ! blockidx%x threadidx%x
           !$acc do parallel, vector(16) ! blockidx%y threadidx%y
           CC 1.0 : 7 registers; 64 shared, 8 constant, 0 local memory bytes; 100% occupancy
           CC 1.3 : 8 registers; 64 shared, 8 constant, 0 local memory bytes; 100% occupancy
           CC 2.0 : 15 registers; 8 shared, 72 constant, 0 local memory bytes; 100% occupancy
```

Tuning the compute kernel

Accelerator VADD Device Code

```
module kmod
 contains
 subroutine vaddkernel(A,B,C)    ! We know array size
  real :: A(:,:), B(:,:), C(:,:)! dimension(2560,96)
  integer :: i,j
!$acc region
!$acc do parallel
  do j = 1,size(A,1)
!$acc do vector(96)
    do i = 1,size(A,2)
      C(j,i) = A(j,i) + B (j,i)
    enddo
  enddo
!$acc end region
 end subroutine
end module
```

Keeping the data on the GPU

Accelerator VADD Device Code

```
module kmod
 contains
 subroutine vaddkernel(A,B,C)
  real :: A(:,:), B(:,:), C(:,:)
!$acc reflected (A,B,C)
!$acc region
   C(:,:) = A(:,:) + B (:,:)
!$acc end region
 end subroutine
end module
```

The !$reflected clause must be visible to the caller so it knows to pass pointers to arrays on the GPU rather then copyin actual array data.

Compiling the subroutine:

```
PGI$ pgfortran -Minfo=accel -ta=nvidia -c vadd.F90
vaddkernel:
    5, Generating reflected(c(:,:))
       Generating reflected(b(:,:))
       Generating reflected(a(:,:))
    6, Generating compute capability 1.0 binary
       Generating compute capability 1.3 binary
       Generating compute capability 2.0 binary
    7, Loop is parallelizable
       Accelerator kernel generated
        7, !$acc do parallel, vector(16) ! blockidx%x threadidx%x
           !$acc do parallel, vector(16) ! blockidx%y threadidx%y
           CC 1.0 : 11 registers; 80 shared, 8 constant, 0 local memory bytes; 66% occupancy
           CC 1.3 : 11 registers; 80 shared, 8 constant, 0 local memory bytes; 100% occupancy
           CC 2.0 : 17 registers; 8 shared, 88 constant, 0 local memory bytes; 100% occupancy
```

Allocating/Deallocating GPU Arrays

Accelerator VADD Device Code

```
subroutine vadd(M,N,C)
  use kmod ! Visibility of !$acc reflected
  real, dimension(:,:) :: A, B, C
  integer :: N
!$acc mirror(A,B)  !device resident clause in 1.3
  allocate(A(M,N),B(M,N))
! C has been mirrored and allocated previously
  A = 1.0
  B = 2.0
!$acc update device(A,B,C)
  call vaddkernel (A,B,C)
  call kernel2 (A,B,C)
  call kernel3 (A,B,C)
  call kernel4 (A,B,C)
!$acc update host(C)
  deallocate( A, B)
 end subroutine
```

Using GPU device-resident data across subroutines

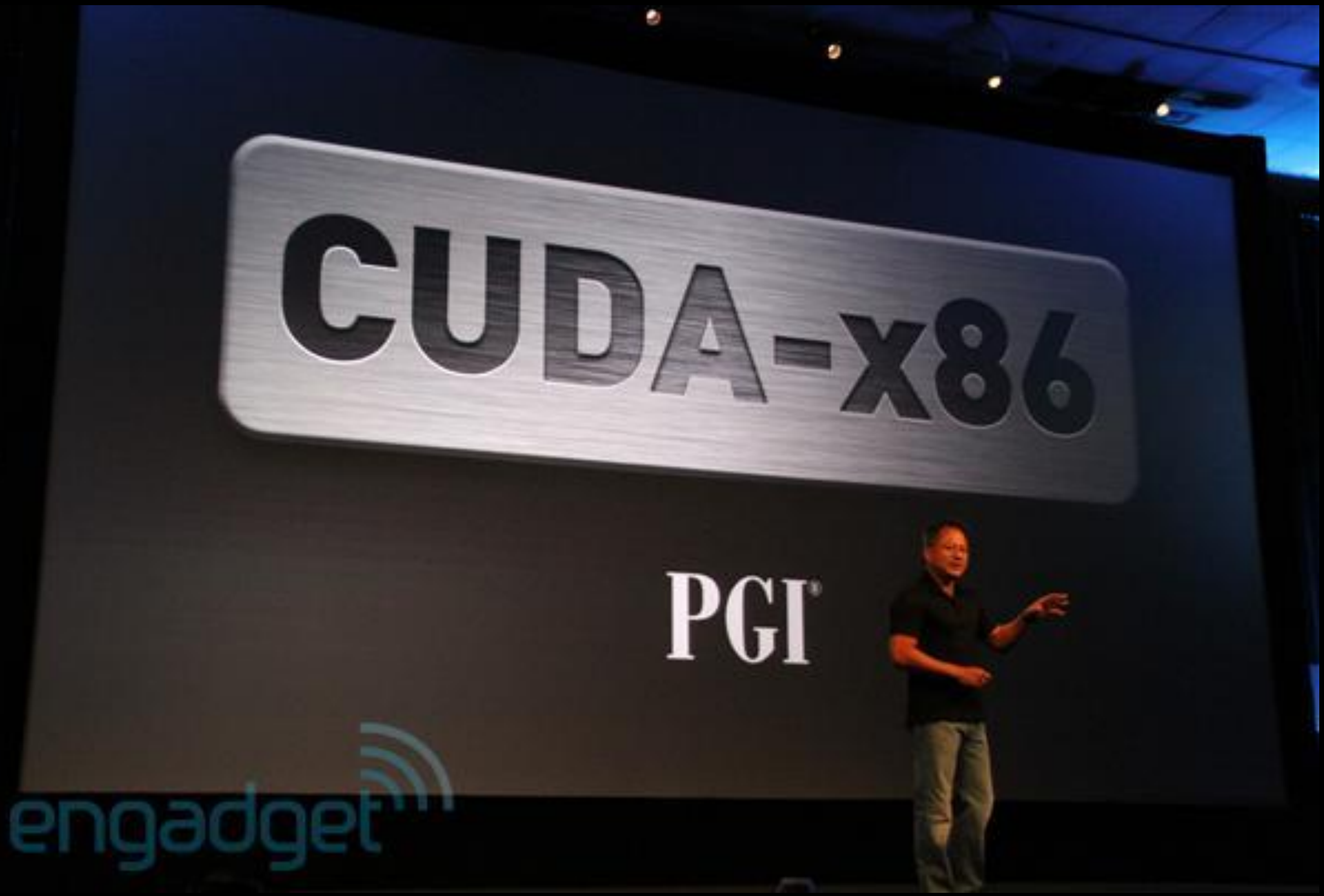
```
subroutine timestep(Input,Result,M,N)
   use kmod ! Make reflected var's visible
   real, dimension(M,N) :: Input,Result

   integer :: M,N
   real, allocatable :: B,C,D
   dimension(:,:) :: B,C,D
!$acc mirror(B,C,D)
   allocate(B(M,N),C(M,N),D(M,N))
   B = 2.0
!$acc update device(Input,B)
   call vaddkernel (Input,B,C)
   ...
   call kernel2 (C,D)
   ...
   call kernel3 (D,Result)
!$acc update host(Result)
   deallocate(B,C,D)
end subroutine
```

CPU Code

```
module kmod
Contains
!
   subroutine vaddkernel(A,B,C)
   real :: A(:,:),B(:,:),C(:,:)
!$acc reflected (A,B,C)
!$acc region
      C(:,:) = A(:,:) + B (:,:)
!$acc end region
   end subroutine
!
   subroutine kernel2(C,D)
   real :: C(:,:),D(:,:)
!$acc reflected (C,D)
!$acc region
      < compute-intensive loops >
!$acc end region
   end subroutine
   ...
end module
```

GPU Code


CUDA-x86
PGI
engadget

```
% pgfortran -help -ta
-ta=nvidia:{analysis|nofma|[no]flushz|keepbin|keepptx|keepgpu|maxregcount:<n>|
            c10|cc11|cc12|cc13|cc20|fastmath|mul24|time|cuda2.3|cuda3.0|
            cuda3.1|cuda3.2|cuda4.0|[no]wait}|host
                   Choose target accelerator
   nvidia          Select NVIDIA accelerator target
   analysis        Analysis only, no code generation
   nofma           Don't generate fused mul-add instructions
   [no]flushz      Enable flush-to-zero mode on the GPU
   keepbin         Keep kernel .bin files
   keepptx         Keep kernel .ptx files
   keepgpu         Keep kernel source files
   maxregcount:<n> Set maximum number of registers to use on the GPU
   cc10            Compile for compute capability 1.0
   ...
   cc20            Compile for compute capability 2.0
   fastmath        Use fast math library
   mul24           Use 24-bit multiplication for subscripting
   time            Collect simple timing information
   cuda2.3         Use CUDA 2.3 Toolkit compatibility
   ...
   cuda4.0         Use CUDA 4.0 Toolkit compatibility
   [no]wait        Wait for each kernel to finish; overrides nowait clause
   host            Compile for the host, i.e. no accelerator target
```

Compute region directive clauses for tuning data allocation and movement

Clause	Meaning
`if (`*`condition`*`)`	Execute on GPU conditionally
`copy (`*`list`*`)`	Copy in and out of GPU memory
`copyin (`*`list`*`)`	Only copy in to GPU memory
`copyout (`*`list`*`)`	Only copy out of GPU memory
`local (`*`list`*`)`	Allocate locally on GPU
`deviceptr (`*`list`*`)`	C pointers in *list* are device pointers
`update device (`*`list`*`)`	Update device copies of the arrays
`update host (`*`list`*`)`	Update host copies of the arrays

Loop directive clauses for tuning GPU kernel schedules

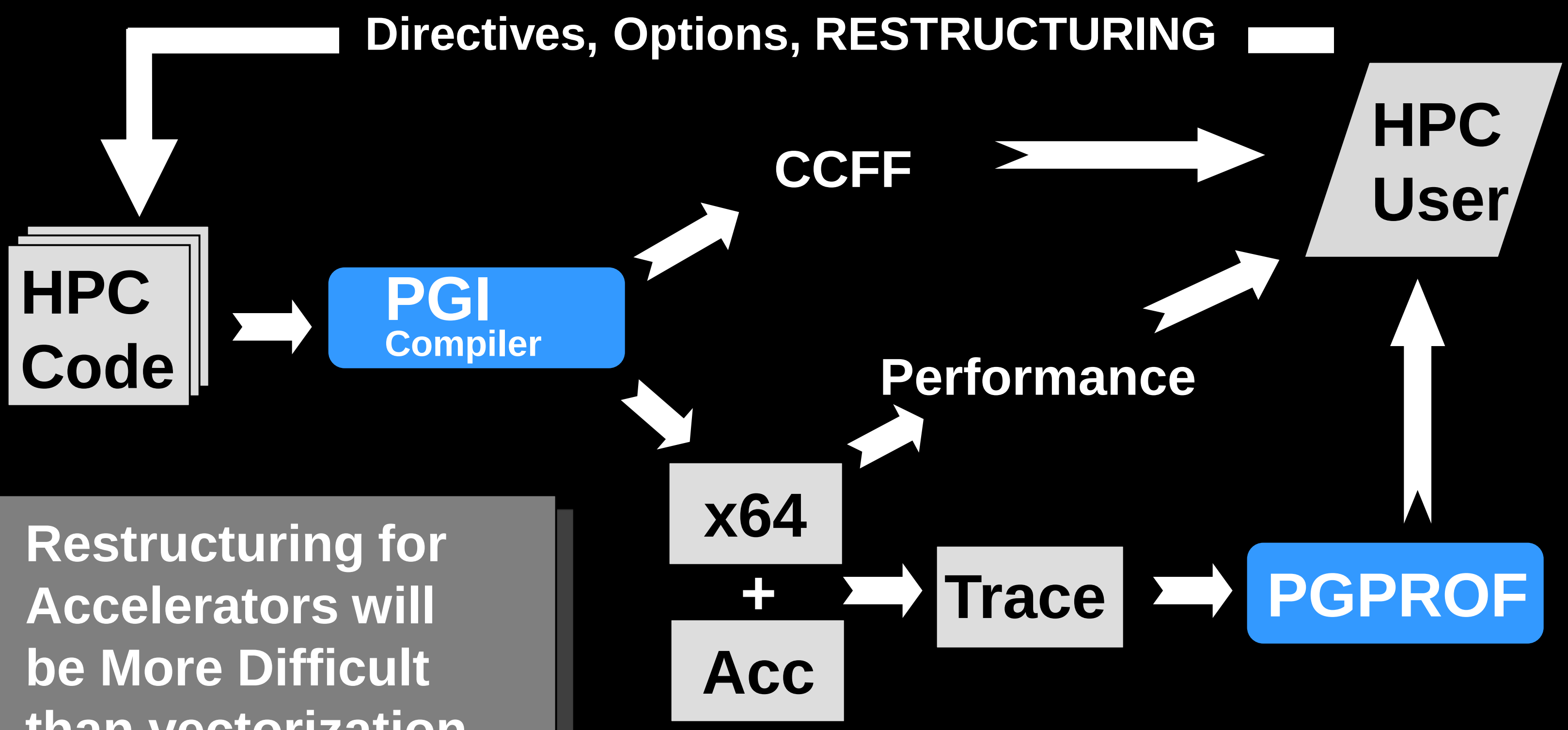
Clause	Meaning
parallel [(*width*)]	Parallelize the loop across the multi-processors
vector [(*width*)]	SIMD vectorize the loop within a multi-processor
seq [(*width*)]	Execute the loop sequentially on each thread processor
independent	Iterations of this loop are data independent of each other
unroll (*factor*)	Unroll the loop *factor* times
cache (*list*)	Try to place these variables in shared memory
private (*list*)	Allocate a copy of each variable in *list* for each loop iteration

Timing / Profiling

- How long does my program take to run?
  - time ./myprogram
- How long do my kernels take to run?
  - pgfortran –ta=nvidia,time
- Environment variables:
- export ACC_NOTIFY=1
- export NVDEBUG=1
- # cuda profiler settings
- #export CUDA_PROFILE=1
- #export CUDA_PROFILE_CONFIG=cudaprof.cfg
- #export CUDA_PROFILE_CSV=1
- #export CUDA_PROFILE_LOG=cudaprof.log

Compiler-to-Programmer Feedback

Incremental porting/tuning for GPUs



Restructuring for Accelerators will be More Difficult than vectorization

Obstacles to GPU code generation

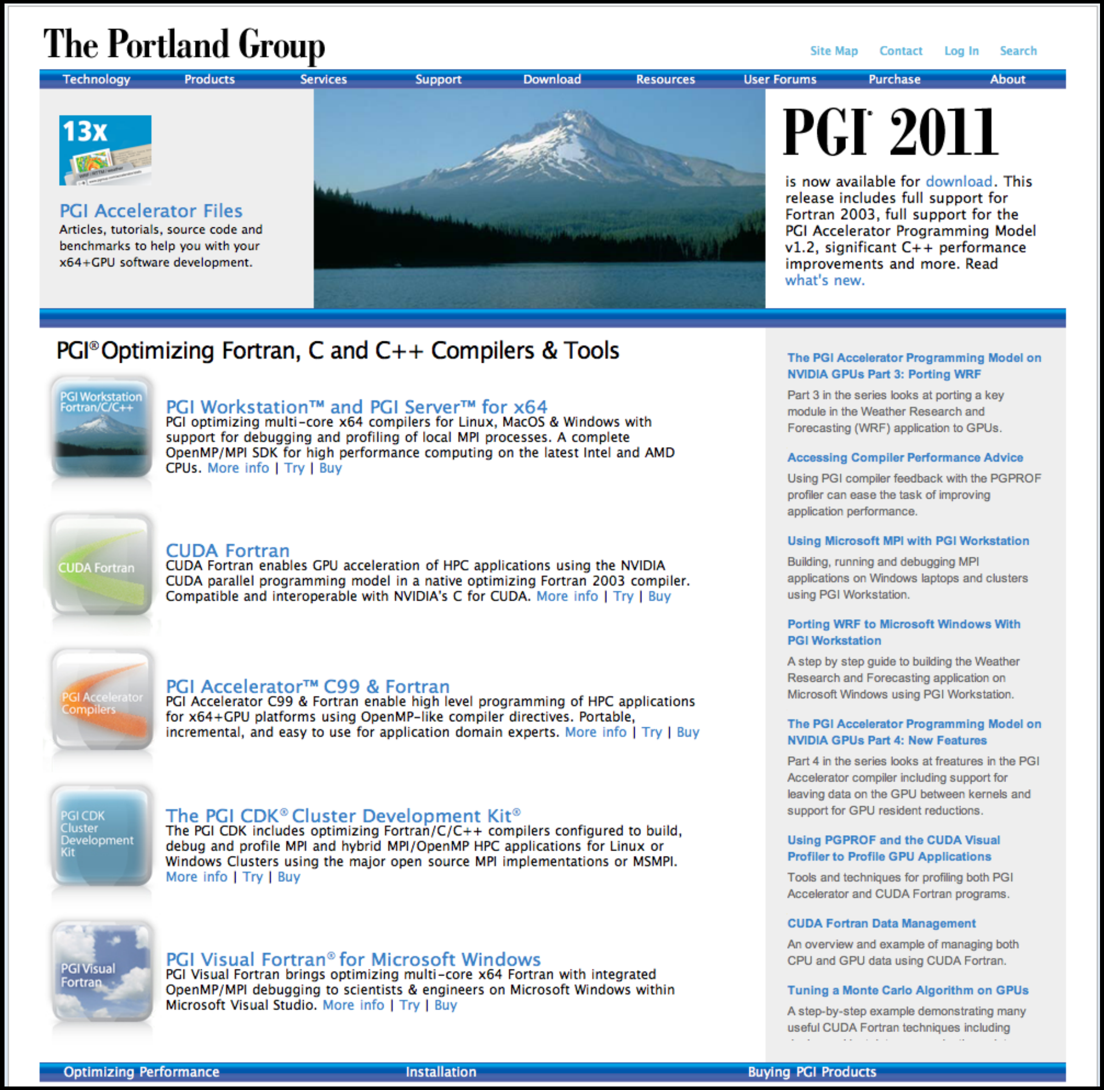
- Loop nests to be offloaded to the GPU must be rectangular
- At least some of the loops to be offloaded must be fully data parallel with no synchronization or dependences across iterations
- Computed array indices should be avoided
- All function calls must be inlined within loops to be offloaded
- In Fortran, the pointer attribute is not supported; pointer arrays may be specified, but pointer association is not preserved in GPU device memory
- In C
  - Loops that operate on structs can be offloaded, but those that operate on nested structs cannot
  - Pointers used to access arrays in loops to be offloaded must be declared with C99 restrict (or compiled w/-Msafeptr, but it is file scope)
  - Pointer arithmetic is not allowed within loops to be offloaded

Evolution of the Directives

- Published Version 1.0 of the PGI Accelerator Directives
  - Intent of publication was to start discussion on standardization process
- Implemented v1.0
- Standardization process started through OMP
- Published Version 1.3 of the PGI Accelerator Directives
- Currently implementing v1.3

PGI

- C99, C++, F2003 Compilers
  - Optimizing
  - Vectorizing
  - Parallelizing
- Graphical parallel tools
  - PGDBG® debugger
  - PGPROF® profiler
- AMD, Intel, NVIDIA, ST
- 64-bit / 32-bit
- PGI Unified Binary™
- Linux, MacOS, Windows
- Visual Studio integration
- GPGPU Features
  - CUDA Fortran
  - PGI Accelerator™
  - CUDA-x86



www.pgroup.com

Reference Materials

- **PGI Accelerator programming model**
  - http://www.pgroup.com/lit/whitepapers/pgi_accel_prog_model_1.3.pdf
- **CUDA Fortran**
  - http://www.pgroup.com/lit/whitepapers/pgicudaforug.pdf
- **CUDA-x86**
  - http://www.pgroup.com/resources/cuda-x86.htm
- **Understanding the CUDA Threading Model**
  - http://www.pgroup.com/lit/articles/insider/v2n1a5.htm